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Confirmation of proton beam bending in graded $Si_{1-x}Ge_x$/Si layers using ion channeling

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A graded composition $Si_{1-x}Ge_x$/Si [001] layer, which has recently been proposed as a method for bending and extracting protons from high-energy particle accelerators, has been studied by angle-resolved ion channeling analysis using focused MeV proton and He^+ beams. Backscattering spectrometry confirms that the composition is linearly graded and a maximum Ge concentration of 0.16 was measured at the epilayer surface. Off-normal planes {111} are curved with respect to the substrate by a total angle of 0.332° and efficient bending of channeled particles along the curved planes and into the substrate is confirmed. © *1999 American Institute of Physics.* [S0003-6951(99)04402-2]

A new application for graded composition $Si_{1-x}Ge_x$/Si layers has recently been proposed for the bending and extraction of MeV–TeV protons from high-energy accelerators.[1] Beam bending is regularly carried out by channeling into bent Si crystals[2,3] because such crystals offer an equivalent magnetic field of up to 1000 T owing to the very short distance over which the bending occurs. However, bent crystals are restricted to a minimum bending length. For this reason, the use of graded silicon germanium for beam bending has attracted considerable current interest in high-energy accelerator laboratories.

For a linearly graded epilayer composition, the Ge concentration as a function of distance d from the substrate/epilayer interface is given by $x(d)=x_s d/h$, where h is the total epilayer thickness, and x_s is the Ge concentration at the epilayer surface. Due to linearly increasing tetragonal distortion, a given set of off-normal planes will curve away from the substrate alignment towards the surface normal with a constant radius of curvature. When a collimated ion beam is aligned with a major crystallographic axis or plane, the ions become channeled[4] and are steered between the atomic rows resulting in a lower energy loss due to a reduced nuclear encounter probability. Providing the radius of curvature R of the graded composition epilayer planes does not fall below the critical minimum radius R_c at which bending dechanneling dominates,[5] most ions which are initially channeled into such curved planes will remain so. They will be steered into the corresponding lattice planes of the Si substrate with little dechanneling at the substrate/epilayer interface. This is because there is no abrupt change in lattice direction owing to the graded nature of the epilayer. Planar rather than axial channeling alignment with the surface is used in such graded samples because the bending efficiency is much higher.

For cubic crystals such as silicon germanium, with a $\langle 001\rangle$ surface normal, an off-normal axis $\langle ijk\rangle$ in the $Si_{1-x}Ge_x$ epilayer is rotated with respect to the substrate axis by an angle $\Delta\psi$ due to tetragonal distortion of the unit cell in the epilayer.[6] This, along with the relationship between tetragonal strain and lattice mismatch, can be used to derive the relationship between the angular rotation and the Ge concentration x:

$$\Delta\psi=\frac{k\sqrt{i^2+j^2}}{i^2+j^2+k^2}\left(\frac{1+\nu}{1-\nu}\right)\times 0.0418x\,, \tag{1}$$

where ν is Poisson's ratio (~0.3).

The radius of curvature for a given set of off-normal planes in a linearly graded composition epilayer is constant, and is given by $R=h\cos\theta/\Delta\psi$, where θ is the crystal tilt angle away from the [001] surface normal direction, and $\Delta\psi$ is the angular rotation between the planes of the Si substrate and the planes at the epilayer surface. As the beam energy is increased, in order for protons to remain channeled within the curved planes, their radius of curvature, and hence, the epilayer thickness h, must also increase for a given rotation angle.[1] The epilayer thickness must not exceed the critical layer thickness[7] beyond which strain is relaxed and misfit dislocations are formed. For graded $Si_{1-x}Ge_x$ crystals required for beam bending in different proton energy regimes it is, therefore, important to be able to accurately measure small strains and lattice rotations from a wide range of epi-

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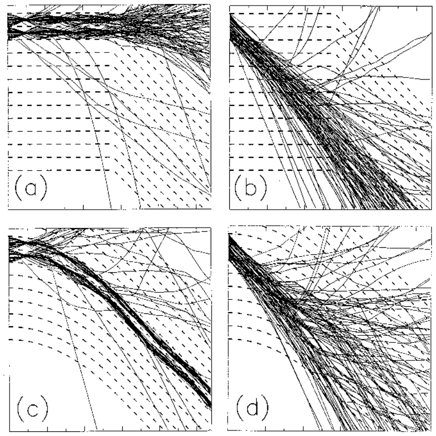

FIG. 1. Simulations showing 100 trajectories of 2 MeV protons in channeling alignment with the surface or substrate (110) planes of the [110] axis in Si bilayers where the first layer is 280 nm thick. The beam is initially distributed over two adjacent (110) planes. Dashed lines represent lattice plane walls. Each box is 3 nm high and 540 nm wide. (a) and (b) show a simple bilayer system with an interface rotation angle of 0.32°. (a) Beam aligned with the surface (110) planes, note the dechanneling at the interface, and (b) beam aligned with the substrate (110) planes. (c) and (d) show an epilayer with curved (110) planes ($R=50$ μm) where the angle between the surface and substrate planes is 0.32°. (c) Beam aligned with surface (110) planes, the beam is bent in the epilayer and channels into the substrate, and (d) beam aligned with the substrate (110) planes. Here, the beam is blocked throughout the curved epilayer planes and cannot channel into the substrate.

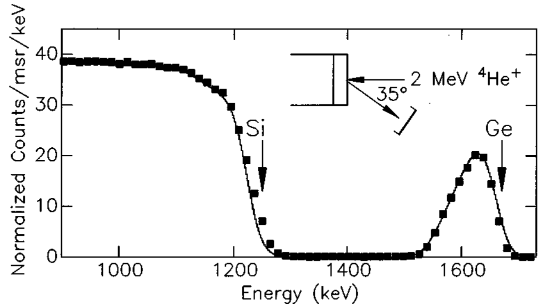

FIG. 2. Backscattering spectrum from the graded $Si_{1-x}Ge_x$/Si sample in a random alignment for a 2 MeV He^+ beam. The squares are data points, the solid line is the fit to the data, showing that the Ge peak is consistent with a linear concentration variation from $x=0$ at the substrate/epilayer interface to $x_s=0.16$ at the epilayer surface. The measured epilayer thickness is 190 nm.

layer thicknesses (~100 nm–1 mm) with a high degree of depth resolution. X-ray diffraction techniques, though highly sensitive to small strains, are limited in analytical depth to considerably less than 100 μm, and, in general, yield an average strain value for the epilayer. Depth-resolved strain measurements from graded layers with x-rays are complex, time consuming, and are possible only with a combination of careful modeling and nonstandard experimental setups.[8]

In this letter, we present ion channeling simulations and results from a graded composition $Si_{1-x}Ge_x$/Si [001] sample which confirm its ability to deflect high-energy protons and conclusively demonstrate that most protons remain channeled through the epilayer and into the substrate.

In the case of uniform heteroepitaxial $Si_{1-x}Ge_x$/Si bilayer structures, a layer of constant Ge concentration x is grown on a Si substrate and an interface rotation (''kink'') angle $\Delta\psi$ is measured.[9] Depth-resolved angular channeling scans from such samples reveal an epilayer surface channeling dip displaced from the substrate dip by $\Delta\psi$.[10] These alignments are illustrated in Figs. 1(a) and 1(b), where 100 trajectories of 2 MeV protons are shown for alignment with the surface or substrate (110) planes (critical angle $\psi_p=0.16°$) close to the [110] axis for a 280 nm Si layer which is rotated by $\Delta\psi=0.32°$ with respect to the substrate. The trajectories were calculated using the Monte Carlo ion channeling program FLUX.[11] In Fig. 1(a), the beam is channeled in the epilayer and most of it dechannels when it encounters the interface since $\Delta\psi>\psi_p$. When the beam is aligned with the substrate planes as in Fig. 1(b), some increase in beam divergence occurs in the epilayer due to scattering, but many protons maintain sufficient alignment with the substrate and are channeled into it.

In contrast, for graded composition samples, those ions that are channeled upon entering the lattice planes at the epilayer surface should remain so throughout the epilayer and be steered into the substrate. This situation is illustrated in Fig. 1(c), where the beam has been aligned with the curved (110) planes ($R=50$ μm, compared with $R_c=6$ μm for 2 MeV protons) at the surface of a 280 nm thick Si layer. The rotation angle between the epilayer surface and substrate planes is again $\Delta\psi=0.32°$. Aligning the beam directly with the substrate planes, as illustrated in Fig. 1(d), reveals that most of the beam is always in a blocking alignment[12] with the curved planes at some depth through the epilayer, which prevents the beam from being channeled into the substrate. Due to the small epilayer thickness, a very small number of particles will avoid the blocking effect and successfully channel into the substrate. However, the only orientations where significant channeling into the substrate occurs are those where the beam is aligned with the crystal planes at the surface of the epilayer, as shown by the simulated trajectories in Fig. 1(c). Therefore, it is only by etching the epilayer off from one part of the sample that the beam can be aligned directly with the substrate, enabling the angular rotation of the epilayer to be measured with respect to the substrate.

The epilayer studied here was grown by molecular beam epitaxy to a nominal thickness of 200 nm, with a nominally linear Ge concentration profile from 0 to 0.15. Rutherford backscattering spectrometry was performed using a 2 MeV He^+ beam to measure the concentration profile and epilayer thickness. Figure 2 shows a random backscattering spectrum from this sample, fitted using RUMP.[13] The epilayer thickness is found to be 190 nm and the Ge peak is consistent with a linear Ge profile, from $x=0$ at the interface to $x_s=0.16$ at the surface. This is the first step in confirming the cause of beam bending by graded layers. The linear concentration profile produces a constant radius of curvature in off-normal planes, with no step in Ge concentration at the epilayer/substrate interface, as found for uniform composition strained layers.[6] Since the epilayer thickness is well below the critical layer thickness for either a constant[7] or graded[1] Ge profile with $x=0.16$, the film is expected to contain no dislocations. This was confirmed using Nomarski optical microscopy.

Angular scans were used to characterize the channeling properties of the sample. These were performed using ion-beam rocking[14,15] on a nuclear microprobe[16] whereby a focused proton or helium beam, with a divergence of <0.05°,

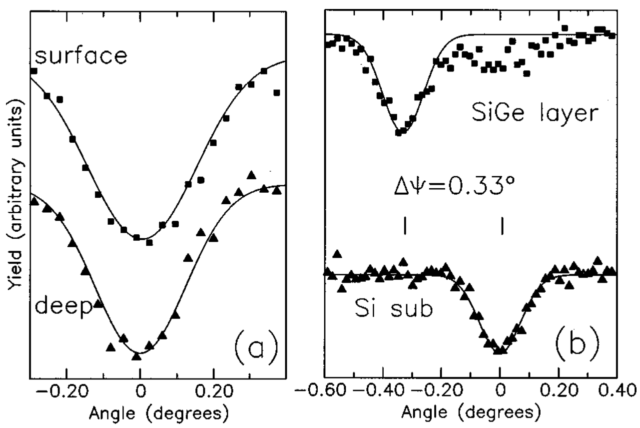

FIG. 3. Angular channeling scans from the graded $Si_{1-x}Ge_x/Si$ sample taken through the (111) planes near the [112] axis. The scans have been offset from each other for clarity. (a) is from the unetched portion using 2 MeV He^+. The "surface" scan is from the surface slice of the Si edge in Fig. 2, corresponding to the first ~40 nm of the epilayer. The "deep" scan is from a slice of the spectrum corresponding to a depth of ~800 nm. (b) shows the Si $K\alpha$ x-ray yield using 3 MeV protons. The beam was rocked over the epilayer to produce the curve labeled "SiGe layer," then translated to an etched region to produce the curve labeled "Si sub." The measured rotation is $\Delta\psi = 0.332° \pm 0.007°$.

is rocked in angle over a small area of the sample surface. Since the sample remains fixed, any mechanical uncertainty due to goniometer rotation is eliminated. This technique has been refined to measure rotations as small as ~0.014° when a proton beam is used (the smaller critical channeling angle compared with helium allows greater sensitivity to small angular rotations). It is, therefore, as sensitive as the catastrophic dechanneling method[17,18] and is applicable to a wider range of crystalline samples, combining the high angular sensitivity and depth resolution which are required in measuring rotation angles as small as 0.5 mrad (≈0.03°) in epilayers which are hundreds of microns thick. Such graded $Si_{1-x}Ge_x/Si$ samples are currently being grown for GeV proton beam bending experiments, and it is important that they can be properly characterized in order to determine their beam bending efficiency.

Figure 3(a) shows two angular channeling scans from the graded $Si_{1-x}Ge_x$ sample performed with a 2 MeV He^+ beam. These were measured with the beam rocked in angle through the (111) planes ($\psi_p = 0.23°$) near the [112] axis (a tilt angle of ~35° from the [001] axis). One scan originates from the surface edge of the backscattering spectrum (see Fig. 2) corresponding to the epilayer surface, and the other from deep within the substrate. There is no observable shift in the position of the channeling minima. This result is evidence that the beam is successfully steered and bent as predicted in Fig. 1(c). In the scans shown in Fig. 3(b), half of the sample's surface was etched to reveal the substrate, in order to measure the angular rotation, as explained above. A 3 MeV proton beam ($\psi_p = 0.13°$, $R_c = 8\,\mu m$) was then rocked on the exposed substrate area, and subsequently, without altering the beam–sample alignment, the beam was translated and rocked over the unetched region. To produce these scans, the Si $K\alpha$ x-ray yield was used because it has a mean production depth of ~20 μm in silicon. This shows that the protons remain well channeled deep into the substrate. As seen in Fig. 3(b), the measured angular rotation between the dips is $\Delta\psi = 0.332° \pm 0.007°$, in good agreement with the value of 0.335° predicted by Eq. (1) for $x = 0.16$ and no strain relief. This conclusively demonstrates that the proton beam is being bent by an angle of 0.332° during the passage through the epilayer, due to the graded composition profile.

In the present work, a graded composition $Si_{1-x}Ge_x/Si$ layer has been analyzed using angle-resolved ion channeling. The angular rotation of the epilayer surface has been measured with respect to off-normal substrate planes by partially etching the sample, and is found to be consistent with the surface Ge concentration measured using backscattering spectrometry, confirming that the epilayer is unrelaxed. On the unetched area, the absence of a shift in the angular position of channeling dips as a function of depth demonstrates that the curved epilayer planes steer MeV protons and He^+ ions into the substrate with a total bending angle of 0.332°, and block them at alignments other than with the surface planes. This letter demonstrates that ion channeling, using a combination of beam rocking and etching, has the angular sensitivity and depth resolution necessary to characterize graded composition $Si_{1-x}Ge_x/Si$ layers where the epilayer is very thick and has a very small rotation angle, as required for GeV proton beam bending experiments.

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